

Viscous and acoustic properties of AlCu melts

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Abstract

© 2016, Pleiades Publishing, Inc. The atomic dynamics of the binary Al100-xCux system is simulated at a temperature $T = 973$ K, a pressure $p = 1.0$ bar, and various copper concentrations x . These conditions (temperature, pressure) make it possible to cover the equilibrium liquid Al100-xCux phase at copper concentrations $0 \leq x \leq 40\%$ and the supercooled melt in the concentration range $40\% \leq x \leq 100\%$. The calculated spectral densities of the time correlation functions of the longitudinal (Formula Presented) (k, ω) and transverse (Formula Presented) (k, ω) currents in the Al100-xCux melt at a temperature $T = 973$ K reveal propagating collective excitations of longitudinal and transverse polarizations in a wide wavenumber range. It is shown that the maximum sound velocity in the $v_L(x)$ concentration dependence takes place for the equilibrium melt at an atomic copper concentration $x = 10 \pm 5\%$, whereas the supercooled Al100-xCux melt saturated with copper atoms ($x \geq 40\%$) is characterized by the minimum sound velocity. In the case of the supercooled melt, the concentration dependence of the kinematic viscosity $\nu(x)$ is found to be interpolated by a linear dependence, and a deviation from the linear dependence is observed in the case of equilibrium melt at $x < 40\%$. An insignificant shoulder in the $\nu(x)$ dependence is observed at low copper concentrations ($x < 20\%$), and it is supported by the experimental data. This shoulder is caused by the specific features in the concentration dependence of the density $\rho(x)$.

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